First-principles calculations of magnetic ultrathin films on surfaces

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Low-dimensional ferromagnetic nanostructures are of fundamental interest. However, ferromagnetism in realistic two-dimensional atomic structures is quite rare, because any finite-temperature magnetic order is prohibited for the isotropic two-dimensional Heisenberg model due to the Mermin-Wagner theorem. In addition, the stability of ferromagnetism in two-dimensional ferromagnetic structures is partially due to the surface magnetic anisotropy. Therefore, it is important not only to examine the magnetic order of the groud state, but also to analyze the magnetic anisotropy. Even though MnN monolayer films on Cu(001) have been reported to have an antiferromagnetic order [1], monolayer films of Mn compounds exhibiting the ferromagnetism have not been reported.

In this study, we demonstrate ferromagnetism in new two-dimensional strcutures on nonmagnetic transition-metal (TM) surfaces [2]. First-principles calculations were performed on the basis of density functional theory with the generalized gradient approximation by the OpenMX code [3]. We have found that MnB/TM(001) and MnC/TM(001) are ferromagnetic, whereas MnN/TM(001) is antiferromagnetic, irrespective of the kind of TM we studied. In Fig. 1, we show the calculated partial density of states (PDOS) of the Mn 3*d* states in MnB/Ag(001). The high PDOS of the nonmagnetic state at the Fermi energy ε_{F} is avoided by the exchange splitting in the ferromagnetic state, which is the characteristic of the itinerant ferromagnetism. With the detailed analysis, we have identified the ferromagnetism in MnB/TM(001) and MnC/TM(001) comes from the double-exchange mechanism, whereas the antiferromagnetism in MnN/TM(001) originates from the superexchange. We also investigated the local magnetic anisotropy energy using second-order perturbation theory [2, 4]. We have clarified the main contributions to the in-plane anisotropy in MnB/Pd(001) as hybridization between Mn and Pd states.

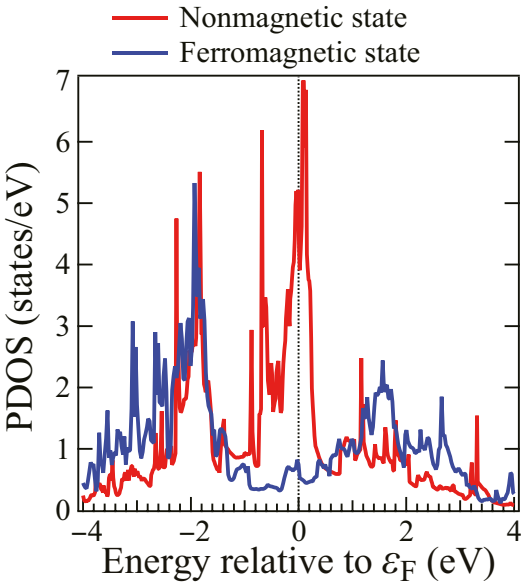

Figure 1: The calculated PDOS of the Mn 3*d* states in MnB/Ag(001) for the nonmagnetic state as well as the ferromagnetic state plotted as the summation of the majority- and minority-spin states.

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